

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -114 °C

Global applicability domain: Inside

Local applicability domain index: 7.58e-01

Confidence level: 6.58e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Propanol</div> <div>Measured: -126</div> <div>Predicted: -114</div>	<div>Image not found</div> <div>Isopropanol</div> <div>Measured: -89.5</div> <div>Predicted: -99.6</div>	<div>Image not found</div> <div>1-Butanol</div> <div>Measured: -89.8</div> <div>Predicted: -95.0</div>
<div>Image not found</div> <div>2-Methyl-1-propanol</div> <div>Measured: -108</div> <div>Predicted: -103</div>	<div>Image not found</div> <div>Allyl alcohol</div> <div>Measured: -129</div> <div>Predicted: -109</div>	